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Numerical modelling of wetting phenomena during melting of PCM

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Abstract

Latent heat thermal energy storage (LHTES) units using phase change material (PCM) exhibit a high thermal capacity, but also a low charging and discharging power. Macro-encapsulation of PCM is one way of enhancing the heat transfer rate in thermal storage units. During encapsulation, the cavity left to reduce mechanical stresses in the macro capsule, locks air. This makes the capsule a multiphase system consisting of immiscible phases namely PCM and air.

Numerical modelling of a PCM capsule enables a detailed understanding of the phase change process of the PCM under the influence of air. In this article, two immiscible fluids PCM and air have been modeled using a continuum surface force (CSF) model in the open source computational fluid dynamics (CFD) software, OpenFOAM. The wetting of the melted PCM on the capsule wall is taken into account by implementing a contact angle boundary condition. The surface tension of the PCM with air is just contributed to the liquid phase of the PCM. The nonlinear enthalpy-temperature relation during the phase change is taken into consideration by a source-based fictitious method. The flow in the solid phase of the PCM is ramped down by considering a high solid viscosity. Experimental results are employed to validate the overall model.

The results obtained from the complete numerical model have shown a great acceptance when compared with experiments. Despite several small deviations in the results, the numerical modelling is a potential tool to optimize the efficiency of thermal storage units.

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Keywords: CFD; PCM; melting and solidification; multiphase; surface tension; convective heat transfer

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1. Introduction

Providing sustainable and clean energy is one of the major contemporary challenges in the field of energy science. Thermal energy storage plays a key role to attain these goals by storing e.g. waste heat released from industries and residential areas. The stored heat can be transported using different mobile carriers or can be stored for later purposes. PCMs can store a comparable high amount of energy per kilogram and are therefore a favorable storage material for mobile applications. Thermal energy storage units containing encapsulated PCM are suitable for mobile applications due to the large heat transfer area leading to a high charging and discharging power. Numerical modelling and simulation of the phase change process of PCM helps to understand the thermal response of the encapsulated storage material. This helps to improve the efficiency of a complete thermal storage.

Numerical modelling of the solid-liquid phase change phenomenon for metallurgical and industrial applications is found empirical. Different techniques exist to model the moving solid-liquid interface in melting and solidification problems. Crank [1] proposed the initial detailed idea to model the moving solid-liquid boundary by solving a diffusion equation. Later, Voller [3] proposed the famous enthalpy method to model convection as well as diffusion during the phase change and also solid velocity ramp down, using the Darcy-Forchheimer equation as a source term in the momentum equation [14]. Gartling [4] proposed a solid viscosity ramp down by implementing a temperature dependent viscosity. This method is called the variable viscosity method (VVM). The first model taking into account the settling of solid PCM and close contact melting was introduced by Asako et al. [5].

Assis et al. [7] modeled the melting of a PCM in a spherical shell using the enthalpy-porosity approach by applying an arbitrary small Darcy constant. Later Rösler [8] extended this method by simulating the more exact melting phenomenon using an enhanced settling method. In this article, a source based enthalpy approach proposed by Swaminathan and Voller [9] is implemented to model the melting of PCM in a capsule. Ramping down the velocity in the solid phase is implemented by the VVM. To account for the two immiscible fluids PCM and air the volume of fluid (VOF) approach is implemented [10]. The surface tension is a material property leading to the elasticity tendency obtained from molecular adhesion of the fluid. Brackbill et al. [6] proposed a continuum approach to model the surface tension between two immiscible fluid phases or fluid-gas phases. In this work the surface tension is modeled using the same CSF approach and the wetting of the PCM fluid is implemented with a contact angle boundary condition. The surface force between the fluid and the gas phase is modeled as a source term in the momentum equation.

The detailed numerical model of a PCM capsule which accounts for phase change, settling of solid PCM, heat transfer and surface tension between PCM and air is modelled in OpenFOAM 2.2.2. Finally the achieved numerical results are compared to experimental results.

Nomenclature

H	Enthalpy, J
F	Force, N
g	Gravitational acceleration, m/s²
L	Latent heat, J/kg
Q	Heat rate, W
c_p	Specific heat capacity, J/(kg·K)
h	Heat transfer coefficient, W/(m²·K)
k	Thermal conductivity, W/(m·K)
p	Pressure, Pa
S	Source term
T	Temperature, K
t	Time, s
u	Velocity, m/s
V	Volume, m³

Greek symbols

θ	Contact angle, Degrees
κ	Curvature, 1/m
ρ	Density, kg/m³
ϕ	Flux, (Arbitrary unit)/(m²·s)
σ	Surface tension coefficient, N/m
μ	Viscosity, Pa·s
γ	Volume fraction of melted PCM
α	Volume fraction of PCM in capsule

Subscripts

g	Gas
l	Liquid PCM
m	Melting
PCM	Phase change material
pc	Phase change
s	Solid PCM
st	Surface tension

2. Numerical model

The complete model consisting of PCM and air in a capsule has been considered as a multiphase system. The governing mass, momentum and energy equations are conserved with segregated fluxes between both PCM and air phases using the volume of fluid method [10]. The volume fraction of PCM α_{PCM} is a marker and cell function used to represent the PCM phase in the geometry. Air in the PCM capsule is represented by α_{Air}, where

$$\alpha_{Air} = 1 - \alpha_{PCM} \, . \tag{1}$$

Modelling phase change in PCM: The PCM phase of the geometry and the phase change behavior of the PCM demands modelling the nonlinear enthalpy-temperature relation. The nonlinear enthalpy-temperature curve can be modeled using a piecewise linear interpolation as shown in the Fig.1. Therefore, the total enthalpy H is defined as a piecewise linear function of the temperature. The total enthalpy can be segregated into latent (H_l) and sensible forms (H_s).

$$H = H_s + H_l. \tag{2}$$

$$H = c_p T + \gamma_l T. \tag{3}$$

In the Eq. 3 c_p is the specific heat capacity of the PCM, T is the temperature and γ_l is the volume fraction of liquid PCM in the finite volume cell. Within the VVM, a consideration of high viscosity in the solid phase restricts the movement of the solid during melting. In this article a single set of mass, momentum and energy conservation equations are solved on a fixed grid for both PCM and air phases. The governing equations in the equation for the advection of the PCM volume fraction [13], is

$$\frac{\partial \alpha}{\partial t} + (\nabla \cdot \alpha_{PCM} u) + (\nabla \cdot \alpha_{PCM}(1 - \alpha_{PCM}) u_r) = 0. \tag{4}$$

Where t is the time, u is the velocity of the PCM in the cell and u_c is the interface relative velocity. The momentum equation of the multiphase system comprising PCM and air as immiscible phases is

$$\frac{\partial \rho u}{\partial t} + \rho u(\nabla \cdot u) = -\nabla p + \mu \Delta u + \gamma_l F_{st} \, . \tag{5}$$

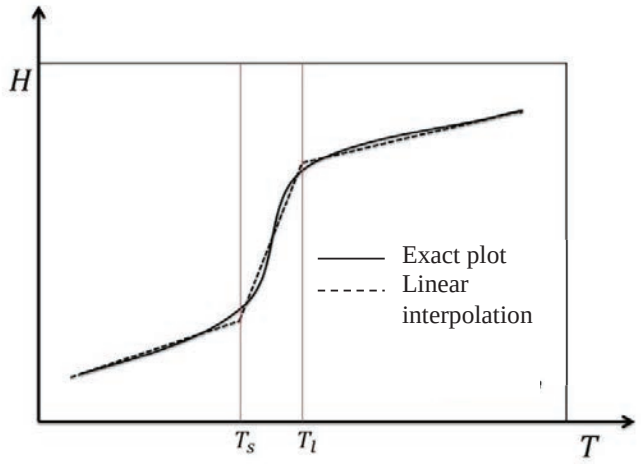

Figure 1: An exact nonlinear enthalpy-temperature curve interpolated using a piecewise linear interpolation function.

All the properties in the governing equations are distributed between two phases PCM and air as

$$\phi = (1 - \alpha_{PCM})\phi_{Air} + \alpha_{PCM}\phi_{PCM}. \quad (6)$$

The total flux ϕ in a cell is distributed between the two phases PCM and air using the volume fraction. In Eq. 6 the total density ρ and the total viscosity μ of the multiphase system are distributed. The velocity u in the cell is also distributed between the phases, but the advection of the interface is understood in detail by Eq. 4 as the velocity depends on the advection of the volume fraction of the PCM (α_{PCM}). In Eq. 5 the source term F_{st} represents the surface tension force between PCM and air in the capsule. This surface tension source term is only present in the liquid PCM phase using the variable γ_l, as the surface tension is a fluid property, and hence can be neglected in the solid phase of the PCM. The surface tension force in the momentum equation is

$$F_{st} = \sigma\kappa\nabla\alpha_{PCM}. \quad (7)$$

Where σ is the surface tension coefficient of the PCM and κ is the curvature of the interface. The term F_{st} is the surface force acting at the interface. The movement of the volume fraction of the PCM in a finite volume cell is as shown below

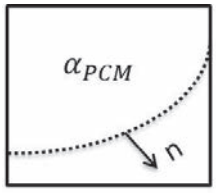

Figure 2: Advection of the volume fraction of the PCM (α_{PCM}) with the normal vector during melting in a finite volume cell.

As shown in Fig. 2 the advection of the interface is calculated through the normal vector (the divergence of the normal vector is the curvature κ in Eq. 7) obtained in the finite volume cell. The advection of the volume fraction is driven by the melting of the solid PCM in the capsule. The increase of the liquid PCM (melting of the solid PCM) is characterized by the energy equation. The governing energy equation of the multiphase system PCM and air is

$$\frac{\partial \rho c_p T}{\partial t} + \nabla \cdot (\rho c_p T u) = \nabla \cdot (k \nabla T) - S_l + T_m \left[\frac{\partial \rho c_p}{\partial t} + \nabla \cdot (\rho c_p u) \right]. \quad (8)$$

Here in Eq. 8 the latent heat source term, S_l is equal to $L \cdot \alpha_{PCM} \left[\frac{\partial \rho \gamma_l}{\partial t} + \nabla \cdot (\rho u \gamma_l) \right]$. The latent heat source term S_l just contributes to the liquid phase of the PCM. In Eq. 8 T_m is the melting temperature of the PCM and k is the thermal conductivity of the multiphase system determined by Eq. 6.

Compressibility: The air in the capsule experiences compression due to the PCM material expansion during melting. To model the physical effect the air in the numerical model is considered compressible and the PCM incompressible. The compressibility of the air is calculated using the ideal gas equation. The melting of the PCM increases the volume of fluid PCM in the capsule which influences the movement of the interface between the PCM and the air. The surface tension between the fluid and the gas phase i.e. liquid PCM and air influence the wetting in the capsule. The contact of the fluid PCM with the capsule wall leads to wetting of the liquid PCM resulting in a capillary meniscus. This physical effect could be modelled by implementing a contact angle boundary condition on the capsule walls. On the wall

$$\cos\theta = \frac{\sigma_{cg} - \sigma_{cl}}{\sigma_{lg}}.$$

Where *c* represents the capsule wall, *l* the liquid PCM and *g* the air phase in a capsule.

Force equilibrium in solid PCM: During melting due to the density difference and buoyancy, the solid PCM experiences settling. The movement of solid into liquid PCM experiencing the detachment from the capsule is called close contact melting [11]. Modelling the force equilibrium on the solid surface influences the solid movement which was first introduced by Asako et al. [5]. Calculating the exact velocity in the solid phase using an iterative approach is a computationally expensive process. Therefore, Asako et al. calculate the settling velocity (u_s) of the solid as a response to the sum of forces acting on the solid. In the VVM, Gartling [4] proposed the consideration of solid as a liquid-solidus i.e. a liquid with very high viscosity. On the other side, for a high viscous flow a settling velocity can be calculated using Stokes flow. Stokes neglected the inertial forces in a momentum equation of a high viscous fluid because of the high resistance offered by the viscosity. This could be applied to the solid PCM to model the settling using the VVM. Stokes law [12] for a very high viscous flow is represented by the equation as below

$$\mu_s \nabla u_s - \nabla p + F_g = 0. \quad (9)$$

In this article Eq. 9 is used to calculate the settling velocity u_s of the solid PCM. The solid PCM in the numerical model is considered as a very high viscous fluid with a viscosity μ_s and F_g is the weight of the solid PCM.

3. Problem Definition

For the problem definition in this article, a cubic capsule geometry in the dimensions of 40 mm x 40 mm x 40 mm is considered. 75 % of the capsule volume is filled with PCM and 25 % with air as depicted in Fig. 3. For air all the material properties depend on the ideal gas equation. The PCM capsule wall has a uniformly distributed heating temperature of T_h = 315 K. A contact angle of θ = 10° has been considered in the simulations by measuring the wettability of the PCM RT35HC. Front and back boundaries of the 3D capsules are considered to be symmetry boundaries.

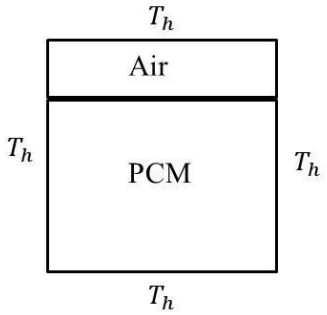

Figure 3: 2D x-y section of a cubical PCM capsule with 75 % PCM and 25 % air

The material properties of the PCM RT35HC of Rubitherm are as follows [8]:

Table 1: Material properties of PCM RT35HC

Material properties	Units	Solid	Liquid
ρ	kg/m³	830.9	778.2
μ	Pa·s	100000	0.0044
c_p	J/(kg·K)	5000	2100
L	J/kg	0	220000
k	W/(m·K)	0.65	0.166
T_{pc}	K	307.65	309.15

4. Experimental setup

In order to validate the numerical model, experiments are employed. Like the numerical one, the experimental setup consists of a cube of 40 mm x 40 mm x 40 mm filled with 75 % PCM and the remaining 25 % with air. Heat exchange in the capsule is employed by a flow of a heated fluid around the capsule. The melting and respectively the melting fronts are captured using a single lens reflex camera. The camera is placed 800 mm away from the opposite to the front boundary. The obtained 2D images are post processed to calculate the melted portion of the PCM and the movement of the PCM-air interface in the capsule.

5. Results and discussions

In the following section the results obtained from the numerical simulations are validated with the experimental results. Different factors like the melting rate, interface advection and the heat flux at the boundaries are analyzed. The surface tension of the PCM RT35HC in liquid form influences the formation of the capillary during melting. Due to the settling of solid during melting, the fluid PCM climbs the solid and spreads near the interface. The settled solid PCM at the bottom of the capsule enhances the heat transfer in the capsule because of close contact melting. The wetting of the melted PCM fluid and the resulting change in volume influences the compression of air in the capsule. The numerical model discussed in this article simulates the wetting of the liquid PCM during melting. As a part of validating the model the interface between the PCM and air is compared with experiments as shown in Fig. 4. Like observed in the experimental results, also in the numerical results the meniscus is formed as soon as melting starts. After t = 2 min the change in meniscus form and curvature is found to be very small. But due to the expansion of the PCM volume during melting the meniscus undergoes translation. The validated meniscus from the numerical model shows a good acceptance with the experimental results.

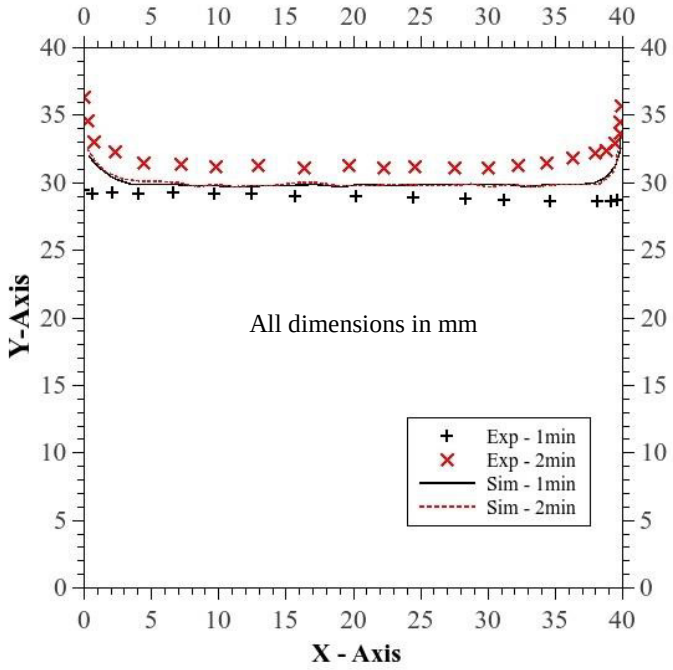

Figure 4: Validating the numerical model with experiments by comparing the interfacial meniscus between PCM and air phase in a PCM capsule.

The surface tension model in the complete model shows a good acceptance apart from the very small deviation because of the translation of the meniscus due to PCM volume expansion. As discussed in the article the solid PCM settles during melting. In Fig. 5 the settling of solid PCM in the numerical model is validated by comparing the solid PCM profile from numerical simulations with the experiments. The settling of solid has shown a very good acceptance in the first two minutes. The solid PCM tends to settle in the similar form as in the experiments. The height and the width of the solid PCM from the numerical simulations after t = 1 and 2 min are validated with the experiments. The width of the solid PCM has a very good acceptance. Because of the faster settling of the PCM in the experiments than in the numerical simulations some deviation in the height occurs. A symmetrical settling of the solid is observed in the numerical simulations. In the experiments the solid PCM experiences different melting forms and cannot be exactly reproduced using a numerical model. However, the interest lies in the melting rate of the PCM and therefore very small deviations in form can be neglected. Fig. 6 shows that the melting rate obtained through simulations shows a good acceptance with the experiments. Therefore, this model can be extended in simulating different capsule forms. The very small difference in slope in Fig. 6 after t = 1 min is due to the statistical starting point of the settling within the experiments which cannot be implemented exactly in the numerical model.

Table 2: Comparing the dimensions of the solid PCM between simulations and experiments.

	Experiments		Simulations	
Time (min)	Height (mm)	Width (mm)	Height (mm)	Width (mm)
1	28.99	39.44	29.04	38.71
2	27.77	38.78	29.23	37.95

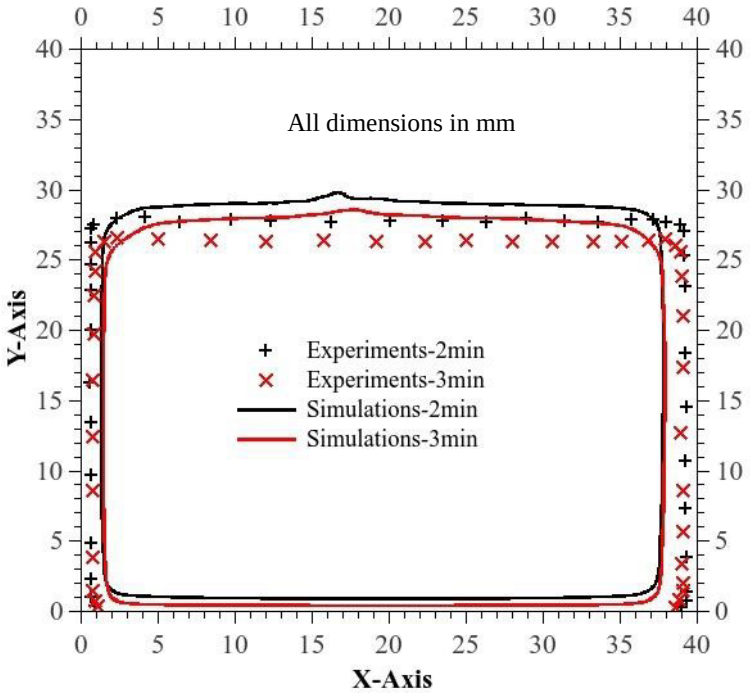

Figure 5: Comparison of the solid PCM from numerical model after 1 and 2 min of melting with the experiments.

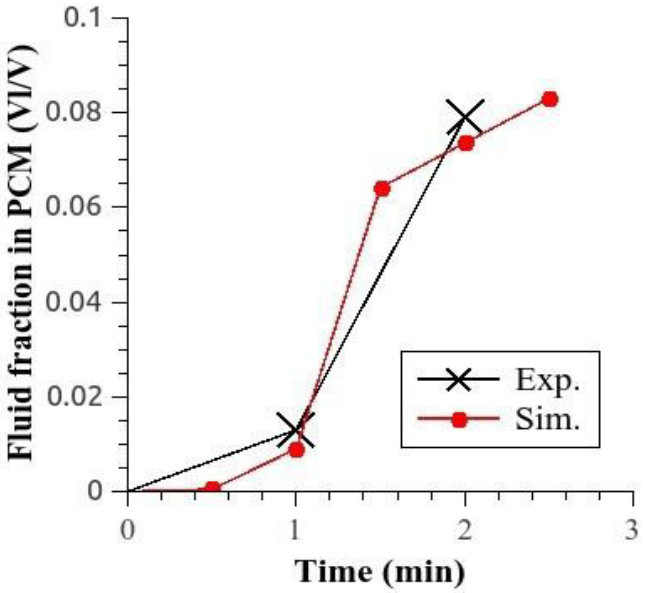

Figure 6: Comparing the melting rate obtained from the numerical simulations with the experiments between the time t = 1 and 3 min.

6. Conclusions

A numerical model for simulating the melting process within a PCM filled capsule is presented in this paper. The numerical model takes account of the two immiscible phases PCM and air using the VOF approach. A source based enthalpy method is chosen to consider the melting enthalpy and the VVM is implemented to switch off the velocity in the solid PCM. To allow the settling of the solid PCM, resulting in close contact melting, Stokes law is applied. The surface tension between the fluid PCM and air is modeled using the continuum surface tension approach. The wetting of the PCM has been implemented in the numerical model through a very acute contact angle as a boundary condition on the capsule wall. The numerical model is validated against experimental results for melting RT35HC in a 40 mm x 40 mm x 40 mm capsule filled with 75 % PCM and 25 % air. Melting rate, solid melting dimension, wetting of fluid PCM and resulting meniscus profile obtained from numerical simulations have been compared with experiments to validate the complete numerical model. This model helps to understand the complete effective phenomena in a PCM capsule. Hence, through numerical simulations with the presented model the efficiency of a heat storage unit can be optimized by varying different parameters like capsule geometry and size, PCM filling portion, material properties and operating conditions. The only challenging factor using this numerical model is the computational stability. The numerical simulations demand a very low courant number approximately less than or equal to 0.25. This could be further optimized for a more stable solution.

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